

CENTER FOR SOLAR AND THERMAL ENERGY CONVERSION

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The goal of the center is to develop the science necessary to elucidate and mitigate energy loss processes in low dimensional, and/or complex nanostructured, organic, inorganic, and hybrid materials for *high efficiency* photovoltaic (PV) and thermoelectric (TE) energy conversion.

PV and TE energy conversion processes are controlled, in part, by the dynamics and interactions between charge carriers and phonons. In PVs, the transfer of energy from photons to electrons occurs through a series of identifiable stages: charge separation, diffusion, charge transfer, charge separation and finally harvesting (Fig. 1). Each stage is characterized by different length scales (0.1 nm-10² nm) and time scales (10⁻⁹-10⁻¹⁵ s) and involves intrinsic energy losses. The interconversion between heat and electricity in TEs is characterized by the figure of merit, ZT.

$ZT = S^2 \sigma T / \kappa$, where S is the Seebeck coefficient, σ is the electronic conductivity and κ is the thermal conductivity, which is controlled by the dynamics of phonons and charge carriers. Enhancing ZT requires decoupling $S^2 \sigma$ and κ through nano-structural design. The research will involve cross-cutting efforts in theory, computation, materials growth/synthesis/fabrication, and physical property measurements, including the use ultrafast optical spectroscopy techniques. This effort will lead to a fundamental understanding of the dynamics and interactions of charge carriers and phonons, which is essential to control and to “tailor” the conversion efficiencies of low dimensional, and/or complex nanostructured, organic, inorganic, and hybrid materials for TE and PV applications.

Research on *inorganic PVs* will focus primarily on low dimensional materials, including arrays of quantum dots and rods. Low dimensional and nanostructured materials show exceptional promise for high efficiency energy conversion. These materials will be fabricated using various self-assembly and patterning strategies, including focused ion beam nanopatterning and selective-array epitaxy. By varying the sizes and the spatial locations of dots and rods in 2D and 3D, the interactions between them may be controlled. The densities of electronic states increase with reduced dimensionality. Moreover, the carrier/phonon interactions, photon absorption/emission, electron/hole recombination and transport are necessarily controllable under conditions of reduced dimensionality and spatial organization. Intermediate band semiconductors, specifically dilute semiconductor alloys, will be considered in this study. Intermediate band- semiconductors are advantageous for overcoming intrinsic losses, associated with thermalization and absorption, experienced by *p-n* junction solar cells. Through a combination of density functional theory (DFT) and molecular simulations, a fundamental understanding of the energy conversion processes will be developed, leading to a series of materials design rules.

Organic PV materials present unique challenges and opportunities for improved efficiency and lower cost. Research will focus on thin-film systems comprising: (1) novel small molecules; (2) conjugated linear chain polymers; (3) dendritic and (4), caged molecules in which the chemical functionalities can be controlled. Self-assembly and patterning strategies will be used to control film morphology (e.g. length scales of phase separation, molecular ordering), which in turn can enhance exciton and charge carrier transport and separation. Molecular dynamics simulations and DFT will accompany chemical synthesis

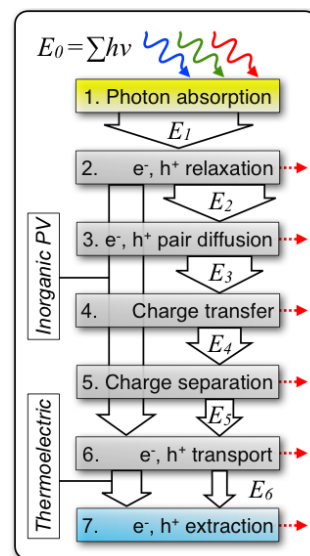


Figure 1: An illustration of the multi-step light-to-electricity conversion processes for organic PV, inorganic PV, and thermoelectrics. The loss mechanisms at each step are also described.

and thin-film processing, and help interpret measurements of ultra-fast energy conversion processes at organic-organic and organic-inorganic interfaces.

The overall aim of our thermoelectrics effort will be to study the fundamental mechanisms that can increase the ZT of a material by maximizing the Seebeck coefficient and electronic conductivity, while minimizing thermal conductivity. Nanostructuring and changes in dimensionality will be used to control carrier and phonon transport, as well as carrier/phonon interactions. Reducing the dimensionality leads to singular features, and enhanced response in the densities of electronic states. Nanostructuring, as well as reduced dimensionality, leads to enhanced scattering of mid-range frequency phonons, which are responsible for heat transport. Conjugated single molecules, specifically metal-molecule-metal junctions, will be investigated for TE applications. Because charge transport is controlled by discrete energy levels, the Seebeck coefficient in conjugated molecules is expected to be large; the thermal conductance is expected to be low due to the significant mismatch between the vibrational spectrum of the molecule and the metal. Simulation and modeling will provide critical insights into the relationship between nano-structure and transport mechanisms, and thereby provide guidance for the structural design of the next-generation TE materials.

The issues associated with nanostructuring TE and PV devices to achieve high energy conversion efficiency are very similar. By manipulating dimensionality of materials structures, their chemical composition, and building block functionality, the dynamics and interactions of phonons and charge carriers can be controlled and studied in both spatial and temporal regimes. In particular, we will utilize advanced ultrafast optical spectroscopy techniques to investigate these processes over a wide range of time scales in different classes of materials. In addition, the molecular and electronic structure of these materials will be determined using a combination of state-of-the art microscopies, x-ray diffraction, and neutron scattering techniques, complemented by detailed computer simulations.

In summary, through combined experimental, theoretical, and computational efforts, we will discover and develop the science associated with energy conversion mechanisms in photovoltaic and thermoelectric devices, fabricated using materials (inorganic, organic, and hybrid organic/inorganic) that possess low-dimensional and/or complex nanostructures. As outcome of our research we will have critically addressed the grand scientific challenges associated with: (1) control of materials processes at the level of electrons; (2) understanding and controlling properties of matter that emerge from the complex correlations of atomic or electronic constituents and (3) characterizing and controlling matter away from equilibrium.

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